

**FUNDAMENTAL STUDIES OF TURBULENT FLOWS WITH
VIBRATIONAL NON-EQUILIBRIUM USING DIRECT NUMERICAL
SIMULATION**

An Undergraduate Research Scholars Thesis

by

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ABSTRACT

Fundamental Studies of Turbulent Flows with Vibrational Non-equilibrium Using Direct Numerical Simulation. (May 2015)

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We study the effects of thermal non-equilibrium (TNE) in particular vibrational non-equilibrium, in decaying turbulence using direct numerical simulation (DNS). The exchange mechanism between molecular vibrational and translational energy modes is introduced using the well-known Landau-Teller approximation. A change in the fundamental cascade is observed with dissipation (ϵ) increasing significantly relative to cases without TNE at time scales of $O(\tau_v)$ where τ_v is the characteristic relaxation time of vibrational energy. This is also found to increase with increase in initial degree of TNE (ΔE_{v_0}) and decrease in τ_v . TNE is also found to increase the decay of turbulent kinetic energy (K). The relative contributions of energy transfer through classical energy cascade and transfer through TNE exchanges can be represented by a new non-dimensional parameter $S_v = \frac{\Delta E_{v_0}}{\tau_v \epsilon}$. S_v can be used to understand DNS data, in particular to distinguish different regimes in the interaction. S_v is also helpful to characterize the time at which dissipation peaks as well as its peak value. Results are compared satisfactorily with experimental evidence available. Turbulence is also observed to affect the transfer of energy from vibrational to translational mode in flows with initial vibrationally hot states. Turbulence accelerates the transfer for small S_{v_0} and decelerates it for large S_{v_0} .

DEDICATION

For Abu and Mummy.
Nothing would be possible without you.

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I would like to express my deepest gratitude to all the people that have made my academic journey possible directly or indirectly. This work would not have existed without the self-less support, love and encouragement from my parents, Abu and Mummy. You have made sacrifices I can only hope that I have the courage to make some day. Nothing that I have ever accomplished or will accomplish in the future would have been possible without you and your tireless hard work to get me started off right in life.

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CHAPTER I

INTRODUCTION

Turbulence is ubiquitous in nature. Turbulent motions are found in a wide array of natural and engineering phenomenon such as mixing of cold cream in a hot cup of coffee, mixing of fuel and oxidizer in a rocket engine and galactic formations. In aerospace applications turbulence is of paramount interest. Development of planetary re-entry systems and future supersonic aircraft depends critically on the understanding of hypersonic flows especially under turbulent conditions. A wide variety of fluid systems, including those associated with turbulent fields, are studied under the so-called continuum assumption without regard for internal structure of the molecules. Atmospheric entry vehicles such as Apollo command vehicle, Orion (currently under development by NASA) fly at speeds exceeding Mach 25 during re-entry. At this velocity the static temperature around the vehicle is approximately 3000 K [1]. At such high temperatures the molecular modes (vibrational, rotational, electronic) need to be considered. Each molecular mode has an equilibrium state defined by local thermodynamics state of the gas [1]. Different molecular modes respond at different time scales to changes in thermodynamic state. The changes may be induced by natural means such as shocks[1] or laboratory means such as laser excitations[2]. When different modes are far from equilibrium, the gas is said to be in thermal non-equilibrium (TNE). Turbulence associated with regimes of thermal non-equilibrium (TNE) is a fundamental phenomenon that has first-order impact on aerospace vehicle performance. In order to achieve an efficient hypersonic vehicle design, it is necessary to understand the fundamental physics involved in both turbulence and TNE and their mutual interaction. We study the effect of vibrational non-equilibrium on decaying turbulent flow. Specifically we study how it interacts with and modifies the other energy modes in turbulence and conversely the effect of turbulence on energy transfers from vibrational to other modes. Excitation of vibrational energy causes the specific heat to become a function of temperature, leading to deviations from calorically perfect to thermally perfect gas.

Motivation and Previous Work

High-temperature flows such as the collapsing gas during the formation of a star, flows behind shock waves that experience large temperature changes can be in various degrees of thermal non-equilibrium. It is also well known that reaction rates can be greatly affected by vibrational non-equilibrium. Thus, it is necessary to understand the fundamental physics involved in both turbulence and TNE and their mutual interaction.

There are numerous studies that suggest a strong interaction between turbulence and TNE. For example, Bertolotti [3] studied the effect of vibrational non-equilibrium in the stability of boundary layers and found that both rotational and vibrational non-equilibrium affect the flow evolution. Rotational non-equilibrium was observed to dampen high frequency instabilities and vibrational non-equilibrium affected the growth of disturbances. However these results were computed only for laminar flows. Most of the studies in the area of TNE and flow interaction are focussed on laminar flows. Very few studies have documented the interaction of TNE and turbulence. In turbulent flows it has been found that a number of thermodynamic and hydrodynamic variables are affected by the degree of rotational non-equilibrium [4] though the effect seemed to be due to an additional bulk viscosity. Liao et. al.[4] studied the effect of rotational non-equilibrium on homogeneous isotropic turbulence. They observed that relaxation of rotational non-equilibrium weakens compressibility after a short initial time. Rotational non-equilibrium was also observed to affect dissipation. The authors noted that the effect on compressibility is more significant for flows with higher Mach numbers that are characterized by stronger compressibility. It has also been experimentally found [2] that vibrational non-equilibrium does have a significant effect on the decay of turbulence. In particular Fuller et. al.[2] found that the decay is faster when the degree of non-equilibrium is increased. The results presented here are in fact applicable to this study and, as we show, help explain the observations in it.

The studies mentioned above focused on limited parameters and lack detailed understanding of the physics involved. Numerical simulations of decaying turbulence with thermal non-equilibrium can help assess the effects of different degrees of non-equilibrium and different modes of evolution

of turbulence. In order to understand the complex two way interaction between turbulence and TNE we use direct numerical simulation (DNS), which aims at resolving all dynamically relevant spatial and temporal scales in the flow. In this paper, we aim to characterize and understand energy exchanges as well as modifications in the evolution of turbulence in the presence of TNE. Gases have multiple thermal degrees including rotational, translational, electronic and vibrational modes. We study TNE at temperatures that are low enough to possess any significant excitation of electronic mode but high enough to interact with others. Rotational-translational modes equilibrate quickly while vibrational relaxation occurs at flow timescales[5]. Therefore in this letter we study decaying turbulent flows with imposed vibrational non-equilibrium with different TNE and flow parameters that govern the evolution of the flow. We study the effect of TNE relaxation on fundamental cascade and decay rate of turbulence. We also address the converse problem of the effect of turbulence on TNE relaxation and the energy exchanges that occur in turbulence and TNE interaction.

Microscopic Structure Of Gases

Gas molecules can be studied by approximating the constituent atoms to be spheres bound by atomic bonds which are approximated by a flexible rod between two atoms. The total degrees of freedom for a molecule depend on the number of constituent atoms. Below we define these degrees of freedom for a diatomic molecule. Molecules with more than 2 atoms have other complex modes about which they may vibrate, rotate or translate

- **Translational energy:** A diatomic molecule can move through space. This motion can be attributed to the center of mass of the molecule. This motion is free in all three dimensions of space and associated with each axis of motion is a translational energy (ϵ'_{trans}). The molecule has 3 geometric degrees of freedom. The velocity component along each axis contributes to the total kinetic energy. Total kinetic energy being a measure of the temperature, the molecule also has 3 thermal degrees of freedom.
- **Vibrational energy:** The atoms of a molecule can vibrate about the axis joining them (flexible rod). Hence the molecule has a vibrational energy (ϵ'_{vib}). This vibrational energy is

transferred between the kinetic energy of the atoms due to the linear motion and the potential energy due to the atomic bond between them. This system can be modeled by replacing the flexible rod by a spring connecting the atoms. The kinetic energy mode adds a single geometric degree of freedom to the diatomic molecule, motion along the joining axis. On the other hand, the total vibrational energy has two modes, kinetic and potential. Therefore there are two thermal degrees of freedom. For molecules with more than 2 atoms, the vibrational modes are varied and much more complex.

- **Rotational energy:** A diatomic molecule may also rotate in space. The rotational energy (ϵ'_{rot}) associated with this mode is dependent on the rate of rotation and the moment of inertia about the axis. Given the small and concentrated distribution of mass of atoms about the internuclear axis of the molecule (flexible rod), the moment of inertia about this axis is negligible. Therefore rotation of the molecule about this axis is meaningless. However the molecule may rotate about other two axis perpendicular to the internuclear axis. These rotations add 2 additional degrees of freedom to geometric and thermal modes.
- **Electronic energy:** Every molecule also has an electronic energy (ϵ'_{elec}) associated with the motion of electrons. The electronic energy is associated with the motion of electrons around the nucleus and the potential energy due to the electromagnetic force between the nucleus and the electrons. The motion itself is complex and therefore the concept of degrees of freedom are not useful [1].

The total energy of a molecule is

$$\epsilon'_{tot} = \epsilon'_{trans} + \epsilon'_{rot} + \epsilon'_{vib} + \epsilon'_{elec} \quad (I.1)$$

$$\epsilon' = \epsilon_0 + \epsilon_{excited} \quad (I.2)$$

Energy in each of the modes is quantized i.e. each mode has discrete energy levels. Each mode has a minimum energy, known as ground state energy (ϵ_{i_0} in eqn. I.2). The modes can be excited from the ground state energy through natural phenomenon (galactic formation, shock waves etc.)

or in the laboratory (laser excitations etc.). The excitation from i^{th} level to j^{th} level depends on the energy gap between the two levels. Based on the mode of excitation, the gap between two consecutive levels may be constant, linear, quadratic in nature. For very high energy levels in a non-linear mode, the levels are close together and seem to overlap [1]. In the absence of external forcing, excitations decay with release of energy through different processes such as light in atomic electronic de-excitation, collisions in gas molecules etc.

Temperatures encountered in hypersonic flight are high enough to excite different energy modes in gases. Further shockwaves (and expansions) in the flow are characterized by strong temperature and pressure changes which modify the ground state energy. Flows with excited energy modes are in thermal non-equilibrium (TNE). The excitations of different modes decay over different time scales. Translational and rotational modes equilibrate very quickly but vibrational relaxation takes place at flow time scales. Numerous studies have shown evidence that TNE affects different flow properties.

Vibrational Non-Equilibrium

In this section we derive the vibrational energy rate equation for a gas. Vibrational energy is transferred between molecules of a gas through molecular collisions. This equation will later be used in conjunction with other fundamental gas equations to study properties of a gas with an active vibrational energy mode.

Consider a diatomic molecule with quantized vibrational energy levels. The quantum mechanical expression for the vibrational energy in i^{th} level is $h\nu \left(i + \frac{1}{2}\right)$ [1]. The population of this level, N_i , changes based on the transfer with levels $i + 1$ & $i - 1$. The population decreases when particles are transferred to other levels and increases when particles from other levels are transferred to this level (i^{th}). Assuming transfers between levels are probabilistic and a collision frequency, we can define a vibrational rate constant $k_{j,i}$ where the transition is from j^{th} to i^{th} level. Then the net rate of change of population of the i^{th} level is

$$\frac{dN_i}{dt} = \sum_{j=-1,1} k_{i+j,i} N_{i+j} - k_{i,i+j} N_i \quad (\text{I.3})$$

Considering a Boltzmann distribution for a gas in equilibrium

$$\frac{N_i^*}{N_{i-1}^*} = \frac{e^{-\epsilon_i/kT}}{e^{-\epsilon_{i-1}/kT}} = e^{-h\nu/kT} \quad (\text{I.4})$$

Since the gas is in equilibrium, the transitions are balanced for both removal and addition of particles

$$k_{i-1,i} N_{i-1}^* = k_{i,i-1} N_i^* \quad (\text{I.5})$$

Combining the above equations, we have

$$k_{i-1,i} = k_{i,i-1} e^{-h\nu/kT} \quad (\text{I.6})$$

Since eqn.I.6 relates the rate constants of two reciprocal processes, it is valid for both equilibrium and non-equilibrium conditions. Using quantum mechanics the rate constants can be expressed in terms of ground state rate constant, i.e.

$$k_{i,i-1} = i k_{1,0} \quad (\text{I.7})$$

$$k_{i+1,i} = (i+1) k_{1,0} \quad (\text{I.8})$$

Combining equations, we have

$$k_{i-1,i} = i k_{1,0} e^{-h\nu/kT} \quad (\text{I.9})$$

$$k_{i,i+1} k_{i+1,i} e^{-h\nu/kT} = (i+1) k_{1,0} e^{-h\nu/kT} \quad (\text{I.10})$$

$$\frac{dN_i}{dt} = k_{1,0} \{ -i N_i + (i+1) N_{i+1} + e^{-h\nu/kT} [-(i+1) N_i + i N_{i-1}] \} \quad (\text{I.11})$$

While studying gas dynamics we are mainly interested in energies rather than populations, we need to convert eqn. I.11 into a rate equation for e_{vib} . For a unit mass of gas

$$e_{vib} = \sum_{i=0}^{\infty} \epsilon_i N_i = \sum_{i=0}^{\infty} (ihv) N_i = hv \sum_{i=1}^{\infty} i N_i \quad (I.12)$$

$$(I.13)$$

Hence

$$\frac{de_{vib}}{dt} = hv \sum_{i=1}^{\infty} i \frac{dN_i}{dt} \quad (I.14)$$

The above equation can further be reduced to the below form

$$\frac{de_{vib}}{dt} = k_{1,0} (1 - e^{-hv/kT}) \left[\frac{hvN}{e^{hv/kT} - 1} - e_{vib} \right] \quad (I.15)$$

Since we are dealing with a unit mass, $Nk=R$, the specific gas constant[1].

$$\frac{hvN}{e^{\theta_v/T} - 1} = \frac{R\theta_v}{e^{hv/kT} - 1} = e_{vib}^{eq} \quad (I.16)$$

where $\theta_v = hv/k$ is the characteristic vibrational temperature and e_{vib}^{eq} is the equilibrium vibrational energy. Then the eqn.I.15 can be re-written as

$$\frac{de_{vib}}{dt} = \frac{1}{\tau_v} (e_{vib}^{eq} - e_{vib}) \quad (I.17)$$

Eqn. I.17 is the vibrational rate equation which relates the time rate of change of e_{vib} to the difference between its instantaneous value and the equilibrium value it is seeking, e_{vib}^{eq} . $\tau_v = \frac{1}{k_{1,0}(1 - e^{-hv/kT})}$ is the vibrational relaxation time. It is famously referred to as the Landau-Teller approximation and is derived assuming a harmonic oscillator for a diatomic gas molecule. A detailed derivation of the above equation can be found in any standard text book on gas dynamics.

Physically eqn. I.17 implies that for gas with vibrational energy greater than the equilibrium energy, the excited particles will exchange energy with Translational-Rotational modes through molecular collisions over a certain time. The energy exchange modifies the gas temperature which in turn changes the equilibrium state of the gas. For $t \rightarrow \infty$, e_{vib} and e_{vib}^{eq} tend to the same asymptotic value.

The vibrational relaxation time (τ_v) itself is a function of temperature and pressure, given by the form[1]

$$\tau_v = \frac{C1}{p} e^{(C2/T)^{1/3}} \quad (I.18)$$

Turbulence

Turbulence is ubiquitous in nature. It involves momentum diffusion, momentum convection and rapid variation of pressure and velocity in space and time. The governing set of equations are the Navier-Stokes equations, which are highly non-linear and notoriously difficult to solve making it a Millennium Grand Challenge[6]. Therefore it is understood through a statistical approach rather than a deterministic one. Certain features of turbulence are

- Irregularity : Turbulent flows are highly irregular.
- Diffusivity : Turbulence leads to an increased homogenization of fluid properties. There is enhanced mixing and increased rates of mass, energy and momentum transports.
- Large Reynolds numbers : The Reynolds number characterizes the strength of the turbulence. High Reynolds numbers, typical of applications, contain a much wider range of scales than low Reynolds number flows.
- Dissipation : Turbulent flows rapidly transfer energy from kinetic mode to internal energy (translational mode of constituent molecules) due to the presence of viscous forces in the flow. In order to sustain turbulent flows, a continuous influx of energy is required.

- Wide range of scales : Turbulent flows are characterized by non-zero vorticity. Large scale vortices are generated whose stretching is responsible for the fundamental cascade of energy from large to small scales. This leads to thinning of vortices in the direction perpendicular to stretching, a direct consequence of volume conservation of fluid elements. As a result larger structures break down into smaller ones until they are small enough to dissipate through viscosity into translational energy. The largest scales are referred to as the integral scales, the smallest are the Kolmogorov scales.

CHAPTER II

DIRECT NUMERICAL SIMULATION

Turbulence is ubiquitous in nature and is considered a very difficult subject in physical sciences and engineering. Well renowned physicist, Richard Feynman, referred to it as the last unsolved problem in classical physics. Advances in understanding and modeling of turbulence are extremely important in a diverse range of applications such as airplane design, galactic formation and combustion. Turbulence is characterized by a wide range of spatial and temporal scales. Turbulent flows have highly non-linear fluctuations in space and time which make it hard to study experimentally. An important tool in studying turbulence is Direct Numerical Simulation (DNS)[7]. DNS solves exact governing equations in turbulence without any assumptions at any scales[7]. The tremendous range of scales in turbulence and their resolution is one of the biggest challenges in DNS. The domain needs to be big enough to capture the largest of the scales, both in time and space, and the grid needs to be fine enough to capture the smallest scales [8]. This creates a need for massive computational power both in terms of speed and memory. The required computational power increases steeply with Reynolds' number which is usually high in desired applications.

The increase in computational power over the last two decades has made it possible to study turbulence in great detail using DNS. The push towards peta scale computing has led to the development of various machines with a large number of parallel processing elements. These resources are exploited with highly efficient and scalable codes with extreme parallelism. In this chapter we provide an overview of the massively parallel code used in this research and also detail the choice of parameters used in the study.

Numerical Scheme and Implementation

Turbulence is governed by the Navier-Stokes equations which express the conservation of mass, momentum and energy. They are represented in compact differential form as below

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \quad (\text{II.1})$$

$$\frac{\partial(\rho u)}{\partial t} + \nabla \cdot (\rho u u) = -\nabla p + \nabla \cdot \tau + f \quad (\text{II.2})$$

$$\frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\rho u E) = -\nabla(pu) + \nabla \cdot q + \nabla(\tau \cdot u) \quad (\text{II.3})$$

As mentioned earlier, turbulence is characterized by wide range of scales. Therefore numerical schemes implemented in the solution of above systems must be able to capture the entire range of scales. In various applications spectral codes satisfy the range of scales but in compressible flow simulations, the appearances of shocklets provides additional challenges which restrict the use of such methods [8]. Additional challenges may be posed by complex geometries and boundary conditions.

An alternative scheme that provides flexibility in the range of scales and geometric features is compact finite differences [8],[9]. These schemes have been widely used in problems with a broadband spectrum such as turbulence where the spectrum expands at higher Reynolds' numbers. We therefore develop a fully compressible solution of Navier-Stokes equations using the mentioned numerical scheme which is 10th order accurate in space. Time discretization is achieved with an RK3 scheme. The code is a massively parallel implementation with hybrid OpenMP/MPI approach [8]. The code has been extensively validated and shown to scale up to over 500,000 cores.

In order to study TNE and additional equation is introduced to model vibrational non-equilibrium. This equation uses the Landau-Teller term derived in the previous chapter as the source term and has the familiar advection-diffusion form [1].

$$\frac{D(\rho e_{vib})}{Dt} = \nabla \cdot (D \nabla e_{vib}) + \rho \frac{e_{vib}^* - e_{vib}}{\tau_v} \quad (\text{II.4})$$

where the terms have same meanings as in chapter I.

In order to have appropriate resolution for TNE processes, an additional CFL_{TNE} condition is used in the code in addition to the familiar viscous CFL. CFL_{TNE} determines the appropriate fineness in the time domain of TNE processes (e.g τ_v). The resultant minimum time is computed by comparing the time scales from viscous CFL and CFL_{TNE} . Such an approach solves all relevant scales not only in turbulence but in TNE as well.

Initial Parameters

A large database of simulations with a wide array of parameters has been developed to study the interaction between TNE and turbulence. The range of parameters includes both flow and TNE parameters. All simulations begin from a fully developed turbulent profile with Taylor Reynolds' number 60. Forcing is stopped at a time ($t=0$) in a fully developed isotropic turbulent flow and TNE is introduced. We consider two turbulent Mach numbers, $M_t = 0.4$ & 0.1 . Different Mach numbers are considered to decouple compressibility effects. The degree of initial thermal non-equilibrium is changed by varying initial vibrational energy, e_{v_0} , and vibrational relaxation time scale, τ_{v_0} .

A full set of initial parameters is listed below

Re_λ	M_t	E_0	E_{v_0}	τ_{v_0}
60	0.4	43.6	1	0.0029
				0.0059
				0.5995
				1.7987
			6	0.0029
				0.0599
				0.1799
				3.5979
			12	0.0029
				0.0299
				0.5995
				1.7987
			20	0.0029
				0.0059
				0.5996
				1.7987
			40	0.0029
				0.0599
				0.1799
				0.7794
				2.3982
				8.3939
			60	0.0029
				0.0059
				0.0299
				0.0599
				0.1799
				0.2698
				0.4497
				8.3937
			600	0.0029
				0.1091
				0.2182
				0.1704
				0.6115
				0.8221

Table II.1
List of initial conditions in DNS database.

CHAPTER III

RESULTS

Energy Exchanges

As described previously simulations begin from a from a fully developed forced turbulent profile. The forcing is terminated at time zero and vibrational non-equilibrium is imposed with the introduction of Landau-Teller approximation in the energy equations. With a given set of vibrational non-equilibrium parameters, the profile is allowed to decay until the vibrational mode reaches equilibrium (Fig III.2).

We start with vibrationally hot states ($e_{v_0} > e_{v_0}^*$) and allow the transfer of energy between different modes. We monitor the energy change in vibrational mode and translation mode (Fig.III.1)by defining their temperatures with the following relationships

$$E = \rho c_v T \quad (\text{III.1})$$

$$E_v = \frac{\rho R \theta_v}{e^{\frac{\theta_v}{T_v}} - 1} \quad (\text{III.2})$$

where c_v is specific heat constant at constant volume, θ_v is the characteristic vibrational temperature and T_v is defined as an effective vibrational temperature, a measure of the energy in vibrational mode. Further more, at long times, both the temperatures approach the same asymptotic value. This indicates that energy is transferred from vibrational mode to translational mode. The transfer is achieved through through molecular collisions.

For a fixed initial vibrational energy (E_{v_0}) the decay time scale is the vibrational relaxation time scale (τ_v). Increasing τ_v slows the decay of energy as expected and vice versa. The decay is however completed on $O(\tau_v)$ as can be seen in fig.III.2. \hat{E}_v is the degree of instantaneous TNE

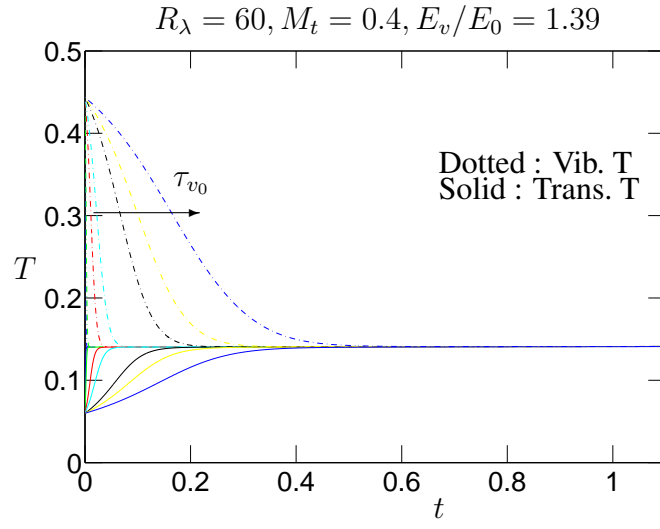


Fig. III.1. Increase in the internal energy consequent with decay of vibrational energy. Mean flow temperature is same as vibrational temperature at $t \rightarrow \infty$. Different colors refer to different characteristic vibrational relaxation time scale (τ_{v_0}).

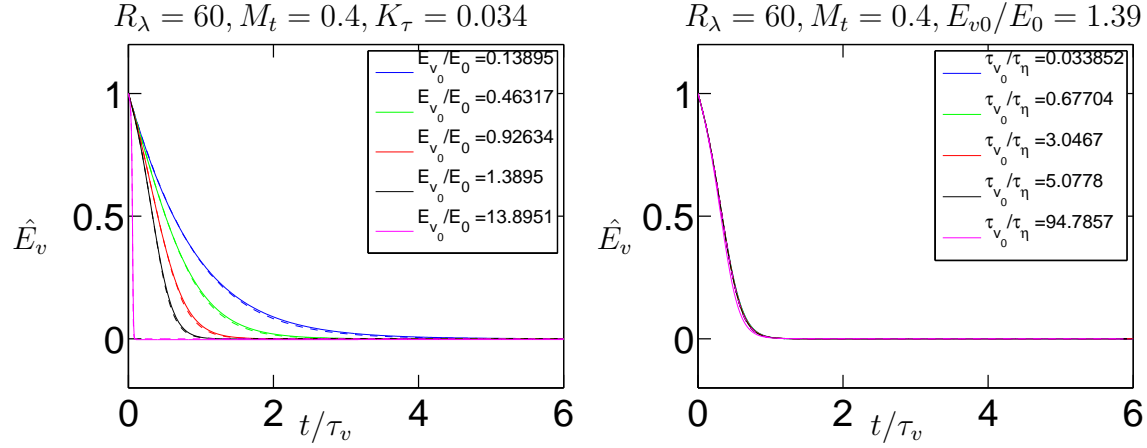


Fig. III.2. Decay of vibrational energy. Solid lines correspond to turbulent decay and dashed lines correspond to laminar decay of TNE for the same set of initial TNE conditions.

as a fraction of the initial degree of TNE. For the initial state of non-equilibrium \hat{E}_v is 1 and at equilibrium it is 0.

$$\hat{E}_v = \frac{E_v - E_v^*}{E_{v0} - E_{v0}^*} \quad (\text{III.3})$$

For a fixed E_{v0} the decay timescale is only dependent on τ_{v0} while as for different E_{v0} , the timescale appears to depend on an additional parameter. Although the decay is always $O(\tau_{v0})$, the actual time in which equilibrium is achieved depends on a parameter that is a function of E_{v0} . The trend seen in fig.III.2 is not completely unexpected for different values of E_{v0} . A larger E_{v0} means a larger energy transfer according to eq. I.17 which results in a larger temperature change. This increased temperature change increases the number of molecular collisions that transfer energy from vibrational mode to the translational mode i.e. reducing τ_v which accelerates the energy transfer.

The decay of TNE affects the fundamental cascade of turbulence. Concurrent with the temperature increase due to vibrational energy decay is the increase in dissipation (ϵ). For cases with TNE a peak in dissipation is observed as seen in fig.III.3. For the same decaying turbulent profile without TNE the dissipation would decay over time as shown in fig.III.4 & This increase in dissipation

indicates a first order effect of TNE on the fundamental cascade of turbulence. The amplitude of the peak increases with decrease in τ_v and increase in E_{v0} . The time of occurrence (τ^*) of the peak in dissipation (ϵ^*) happens on TNE time scales, $O(\tau_v)$. The increase in dissipation is attributed to the increase in viscosity. Viscosity is proportional to temperature and increasing temperature due to vibrational energy decay(Eqn. III.4) increases viscosity.

$$\frac{\mu}{\mu_0} \approx \sqrt{\frac{T}{T_0}} \quad (\text{III.4})$$

$$\epsilon \propto \mu \quad (\text{III.5})$$

Increasing τ_v slows the transfer of energy from vibrational to rotational-translational mode and therefore the peak is delayed and conversely decreasing τ_v advances the peak. The increase in dissipation was observed experimentally by Fuller et. al.[2] in flows with vibrationally excited modes. The questions that we would like to answer are

- What are the dynamics of this turbulence-TNE interaction?
- What parameter(s) govern this interaction?

Regimes of the decay: the non-dimensional parameter S_v

In order to answer the above mentioned questions, different 'active' energy modes in the flow are considered. Turbulent flows are characterized by turbulent kinetic energy dissipation, ϵ , as described by the eqn.III.6. In the presence of TNE, an additional mode is active, in our case vibrational mode, E_v , that interacts with translational mode according to Landau-Teller relaxation as described in eqn.III.7. Both dissipation and vibrational relaxation interact with the translational mode, E , as described in eqn.III.8.

$$\frac{d\langle K \rangle}{dt} = \langle \epsilon \rangle \quad (\text{III.6})$$

$$\frac{d\langle E_v \rangle}{dt} = \left\langle \frac{\rho}{\tau_v} (e_v^{eq} - e_v) \right\rangle \quad (\text{III.7})$$

$$\frac{d\langle E \rangle}{dt} = -\left\langle \frac{\rho}{\tau_v} (e_v^{eq} - e_v) + \epsilon \right\rangle \quad (\text{III.8})$$

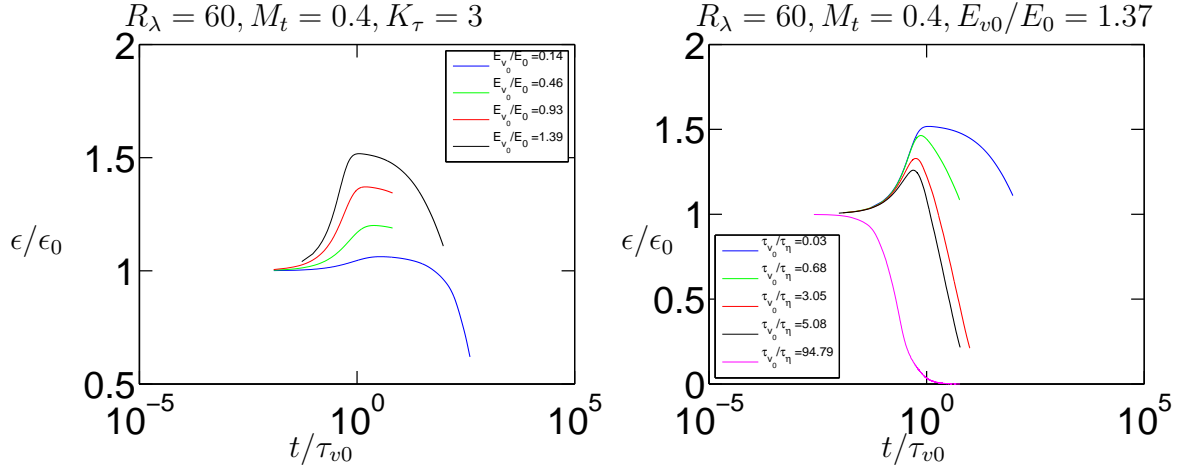


Fig. III.3. Local Maxima are observed in dissipation for simulations with TNE. The amplitude of maxima increases with increase in E_{v0} and decrease in τ_{v0} .

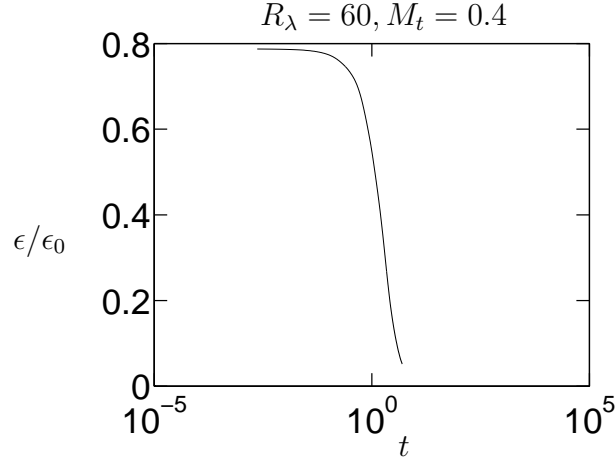


Fig. III.4. Dissipation in a purely turbulent flow decays over time.

Therefore one of the parameters can be the ratio of the two competing processes, S_v .

$$S_v = \frac{|E_v^* - E_v|}{\tau_v \epsilon} \quad (\text{III.9})$$

The parameter S_v is the relative importance of turbulent cascade and TNE. $S_v \gg 1$ is a flow regime where TNE affects turbulent dynamics and $S_v \ll 1$ is a flow regime where turbulent cascade is

largely unaffected by TNE. The parameter can also be derived by normalizing the flow dynamics equation (eqns.III.6, III.7, III.8) by mean dissipation, $\langle \epsilon \rangle$.

$$\frac{1}{\langle \epsilon \rangle} \frac{d\langle E \rangle}{dt} = -\frac{1}{\langle \epsilon \rangle} \left\langle \frac{\rho}{\tau_v} (e_v^{eq} - e_v) \right\rangle + 1 \quad (\text{III.10})$$

$$\frac{1}{\langle \epsilon \rangle} \frac{d\langle E \rangle}{dt} = -S_v + 1 \quad (\text{III.11})$$

The initial value of S_v is successful in predicting the peaks in dissipation(ϵ^*) for flows dominated with TNE as well as time of occurrence (τ^*) of the peak. First plot in fig.III.5 shows the fractional increase in dissipation ($\langle \epsilon \rangle$) as a function of the initial value of S_v . For small degrees of TNE, $S_{v0} < 15$, there is essentially no increase in dissipation as TNE does not affect turbulent cascade for small S_{v0} . For large degrees of non-equilibrium, $S_{v0} > 15$, turbulence is interacting with TNE and increase in dissipation is observed. For extremely large values of S_{v0} TNE time scales are much shorter than turbulent time scales and the increase in dissipation asymptotes. In this regime, TNE affects the turbulent cascade at the onset of the decay. As expected, higher vibrational energy produces larger temperature change in the flow and therefore a larger change in dissipation is observed (eqn.III.4). The asymptotic value of the increase in dissipation can therefore be predicted by assuming an energy balance

$$\langle \rho e_0 \rangle + \langle \rho e_{v0} \rangle = \langle \rho e_\infty \rangle + \langle \rho e_{v\infty}^* \rangle \quad (\text{III.12})$$

$$(\text{III.13})$$

or

$$\langle E_0 \rangle + \langle E_{v0} \rangle = \langle E_\infty \rangle + \langle E_{v\infty}^* \rangle \quad (\text{III.14})$$

The terms on the left side of the equation are known initial conditions and the terms on the right define the final equilibrium conditions which depend on temperature, T . The energy balance assumes that TNE time scales are much faster than turbulent time scales ($\tau_v \gg \tau_\eta$) and the decay of TNE is achieved instantaneously ($\tau_v \rightarrow 0$). Such a decay produces a temperature change (eqn.III.1) which

increases viscosity of the flow. The increase in viscosity increases dissipation (eqn.III.4). The above equation (eqn.III.12) can be solved for the final temperature T_∞ of the flow and the resulting dissipation can be calculated using eqn.III.4, where $T = T_\infty$. The solution is plotted in fig.III as the dashed line. It is clear that DNS data agree very well with the expected value. Therefore we can conclude that the increase in dissipation is due to temperature change caused by vibrational energy decay.

In the second plot of fig.III.5 the time of the peak (τ^*) is measured as a function of S_{v_0} . For small values of $S_v, S_{v_0} < 15$, the initial value of dissipation is the maximum value as TNE does not affect the turbulent cascade. As the degree of non-equilibrium is increased (S_{v_0}), TNE and turbulence interact and peaks in dissipation are observed. Increasing S_{v_0} increases the rate of energy transfer and therefore the peak in dissipation occurs at earlier times i.e. $\tau^* \rightarrow 0$. For large values of S_{v_0} , the time of occurrence of peak asymptotically approaches zero as the energy is transferred from vibrational mode instantaneously resulting in an instantaneous change in temperature. Slower energy transfer delays the peak.

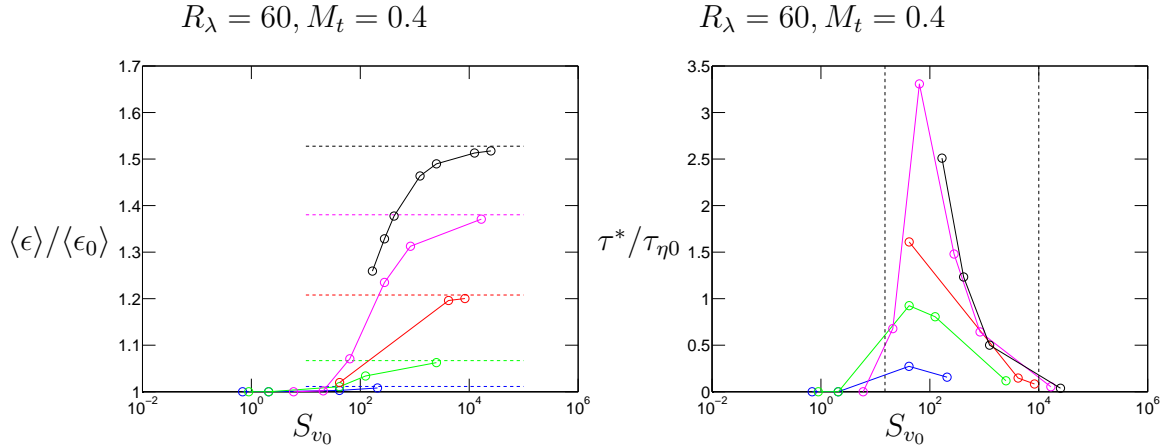


Fig. III.5. Peaks in dissipation are observed for simulations with $S_{v_0} > 15$. For a fixed E_{v_0} , ϵ shows asymptotic behavior with decreasing τ_v or increasing S_{v_0} . Different colors are different E_{v_0} as in fig.III.2. Circles are DNS data and dashed line are theoretically predicted asymptotes.

The increase in dissipation has the effect of increasing the decay of turbulent kinetic energy III.6. We monitor the decay of turbulent kinetic energy (K) for a purely turbulent profile and the decay

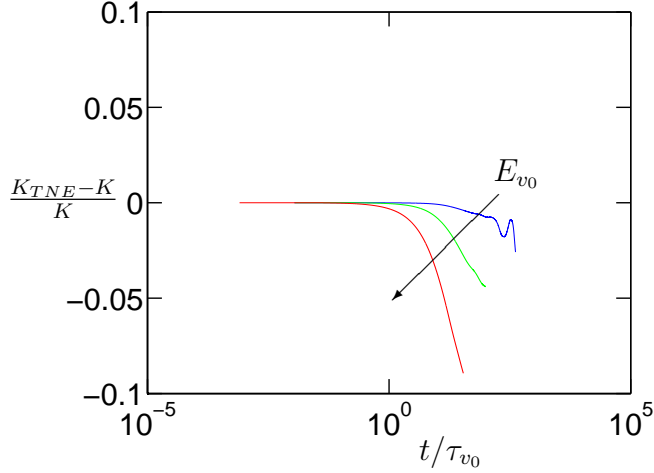


Fig. III.6. Change in TKE (DNS). Direction of arrow indicates increase in E_{v_0} .

of K_{TNE} in the same turbulent profile in the presence of TNE. It is observed (fig.III.6) that the decay is accelerated by increasing the degree of initial non equilibrium (E_{v_0}). Fuller et.al. [2] observed experimentally that increasing the amount of vibrational energy accelerated the decay of kinetic energy. We can estimate the $S_{v_0} \sim O(10^4)$ in their data that corresponds to an a degree of non-equilibrium in the magenta curve in fig.III.5. Our theory expects a 40% increase in dissipation for such a flow. Fuller et. al.[2] reported a 46% increase in dissipation of K which agrees very well, within experimental error bounds, with our expected value.

S_v also helps define regimes in the decay. S_v is a dynamic quantity that changes in time as the vibrational energy decays. As reported in earlier sections, at early times, vibrational energy decay occurs $\sim O(\tau_v)$ as seen in fig.III.2. However near equilibrium, S_v is low therefore turbulent time scales become more important. The decay near equilibrium occurs at turbulent time scale, such as eddy turnover time (T_E) which is much slower than τ_v as seen in fig.III.7. An interesting feature to note is that \hat{E}_v can be negative for large values of $S_{v_0} \sim O(10^4)$. This indicates that vibrational decay overshoots equilibrium and flows that started as vibrationally hot, become vibrationally cold! The amount of overshoot increases with increasing S_{v_0} . This regime of the decay is turbulence

dominated and the relaxation is much slower than earlier. This indicates a correlation between E_v, E_v^* & τ_v . It also means that in turbulent flows with TNE, equilibrium is achieved when

$$\left\langle \frac{E_v}{\tau_v} \right\rangle = \left\langle \frac{E_v^*}{\tau_v} \right\rangle \quad (\text{III.15})$$

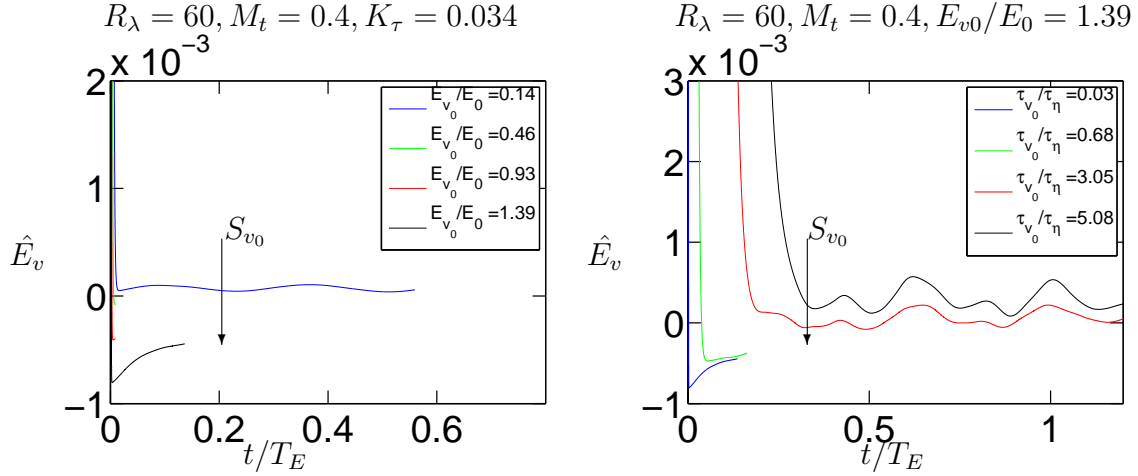


Fig. III.7. Decay of vibrational energy. Solid lines correspond to turbulent decay and dashed lines correspond to laminar decay of TNE for the same set of initial TNE conditions. Arrows indicate increasing S_{v0} .

A model for the decay

Results in the previous sections demonstrate the effect of TNE on turbulence and also the effect of turbulence on TNE decay. We further investigate the effect of turbulence on TNE . In order to quantify such effects, a laminar model of the decay is proposed based on the results in section III. A laminar flow with TNE is governed by the following equations

$$\frac{dE_v}{dt} = \frac{E_v^* - E_v}{\tau_v} \quad (\text{III.16})$$

$$\frac{dE}{dt} = -\frac{E_v^* - E_v}{\tau_v} \quad (\text{III.17})$$

The above system is highly non-linear but can be solved numerically to study the evolving terms, E_v and E . These equations were solved using an RKDP method - an explicit fourth-order Runge-Kutta method with variable step size for error control.

The solution is plotted in fig.III.2 as dotted lines. The decay of energy in a laminar model is similar to turbulent decay at large degrees of non-equilibrium. However near the equilibrium, the behavior is significantly different. The decay of energy in a laminar flow occurs purely at TNE time scales and there are no separate regimes as found in turbulent flows. The decay is complete when $E_v^* = E_v$ as opposed to turbulent case as eqn.III.15.

We focus on the total time scale of decay as a measure for the effect of turbulence on TNE . Effective time scales, τ_L & τ_T , are defined as the time length of non-equilibrium in laminar and turbulent flows respectively.

$$\tau_i = \left(\frac{dE_v}{dt} \right)_{t=0} \int_0^\infty \frac{E_v^* - E_v}{\tau_v} dt \quad (\text{III.18})$$

The ratio of two effective time scales is a mixing ratio (r_m). $r_m > 1$ means the transfer of energy from vibrational mode to rotational-translational mode is accelerated and $r_m < 1$ means the transfer is inhibited.

$$r_m = \frac{\tau_L}{\tau_T} \quad (\text{III.19})$$

It is observed that energy transfer is accelerated for small values of S_{v_0} and decelerated for large values of S_{v_0} . Both E_v and K have the effect of reducing vibrational relaxation time scale (τ_v) by increasing temperature eqn.I.18. Since K is only present in turbulent flows, turbulent flows experience a further shortening of τ_v as compared to laminar flows. The net effect is an accelerated decay of TNE in turbulent flows i.e. $r_m > 1$. However for very large values of S_{v_0} there is an increased overshoot of E_v with respect to E_v^* as described in previous section. The decay of TNE in the overshoot region happens at turbulent time scales which are much slower than TNE time scales. Therefore this slow region dominates the earlier acceleration experienced in TNE decay

and has an over all effect of slowing down the total decay time scale. Therefore $r_m < 1$ for large values of S_{v0}

$$R_\lambda = 60, X : M_t = 0.4, o : M_t = 0.1$$

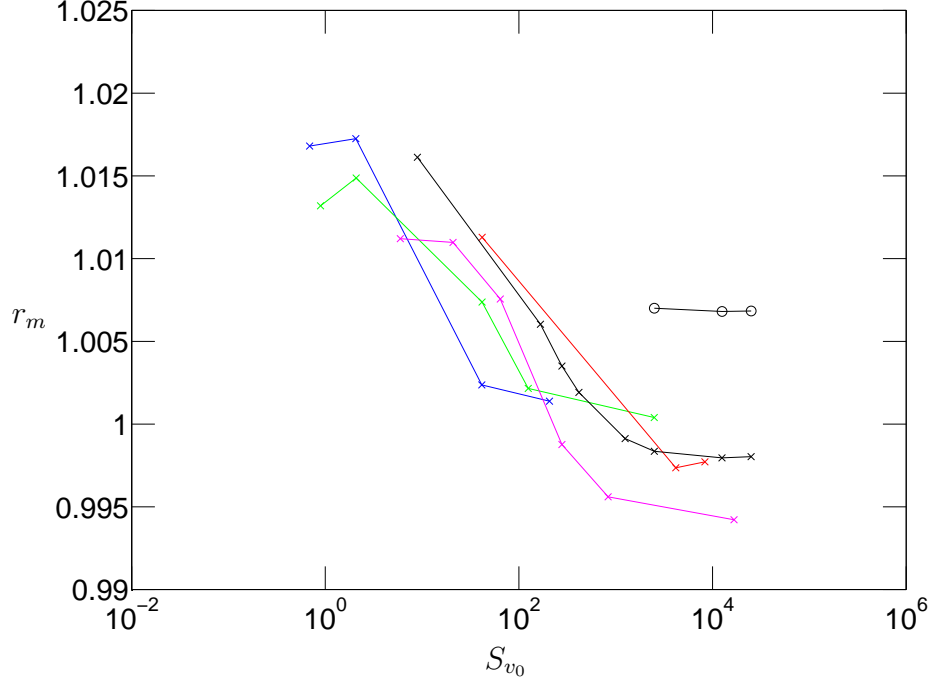


Fig. III.8. Effect of S_{v0} on r_m . Turbulence accelerates the decay for low S_{v0} and decelerates the decay for high S_{v0} .

For smaller turbulent Mach number (M_t), the compressibility is reduced and temperature fluctuations are smaller [10]. Therefore turbulence is weak even at high S_{v0} and the decay of TNE is faster at low M_t (fig.III.8).

CHAPTER IV

CONCLUSIONS

We studied the interaction of TNE and turbulence to ascertain the underlying energy exchanges and parameters that govern such dynamics. Turbulence in the presence of TNE is an important component in a broad spectrum of natural phenomenon such as galactic formations and engineering applications such as hypersonic vehicle design. Yet there is a lack of understanding in the interaction between turbulence and TNE. Certain experimental work hints at their interaction but lacks the understanding of underlying physics and governing parameters. This work is an essential starting point in understanding this interaction.

We performed direct numerical simulations of decaying turbulent flows with imposed vibrational non-equilibrium. A clear interaction between turbulence and TNE is observed. TNE affects the classical turbulent cascade by changing dissipation. Local maxima (ϵ^*) are observed in turbulent flows with thermal non-equilibrium. The amplitude of the maximum increases with increasing initial vibrational energy (E_{v_0}) and decreasing vibrational characteristic relaxation time scale (τ_v). The amplitude of the peak asymptotes for a given E_{v_0} by decreasing τ_v . An important parameter governing this dynamics is the relative importance of TNE and turbulent cascade, S_v . S_v is successful in characterizing the peaks in dissipation and the time of occurrence of peak (τ^*). At early times vibrational energy decays $O(\tau_v)$ and near equilibrium the relaxation occurs at relatively slower turbulent time scales. Turbulence is also observed to affect the decay of TNE in the flow in comparison to laminar decay. For small values of S_{v_0} turbulence accelerates the transfer of energy from vibrational to translational-rotational mode while as for very large values of S_{v_0} turbulence hinders the relaxation of TNE. The effect is more pronounced at high turbulent Mach numbers due to increased compressibility.

Although this work characterizes turbulence-TNE interaction for a wide spectrum of TNE parameters, further work needs to address the effect of flow parameters on TNE. An initial study on the effect of M_t has been carried out in this work, but a detailed study including a wider range of

flow parameters such as M_t , Reynolds numbers (R_λ) etc. is warranted. Further work also needs to address some questions regarding laminar decay. The actual decay time of TNE is observed to depend on E_{v_0} and E , both in turbulent and laminar decays. This hints at additional parameters that govern the dynamics and needs further investigation.

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